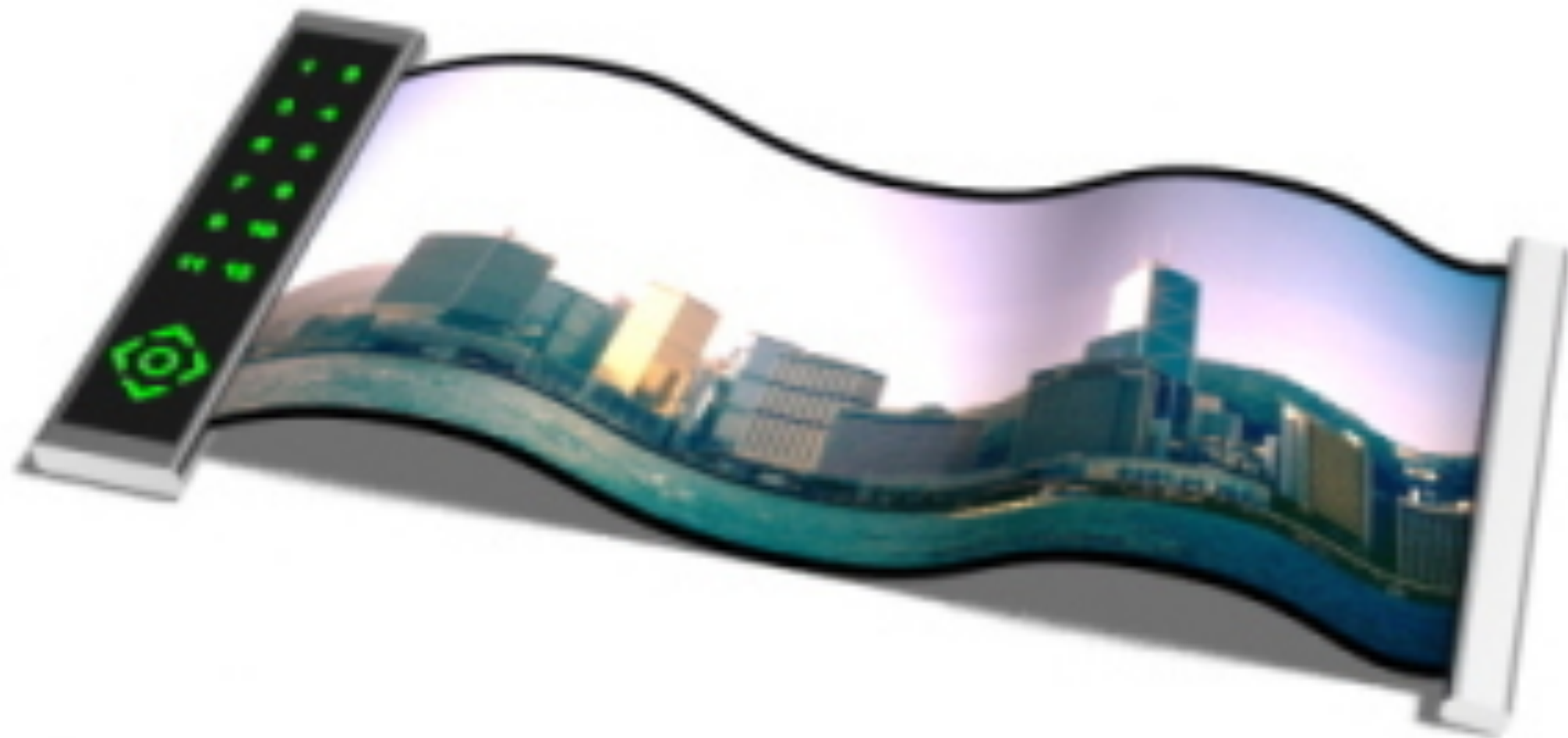# Computational Materials Design
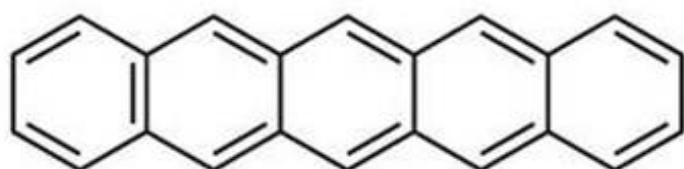
Project 3

Machine learning for predicting transfer integrals in organic semiconductor
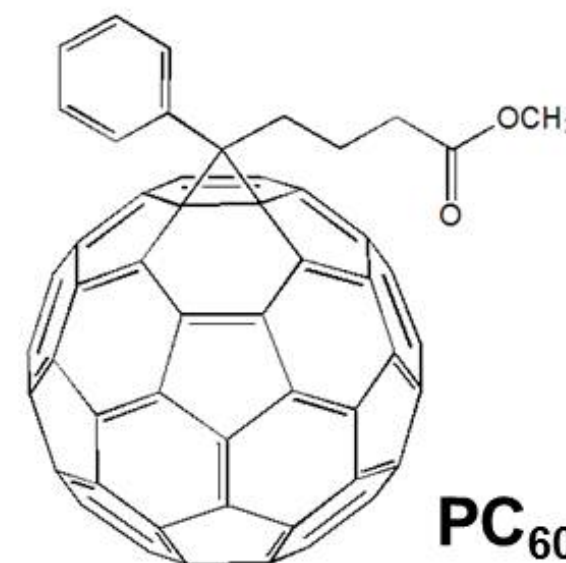
Organic semiconductors
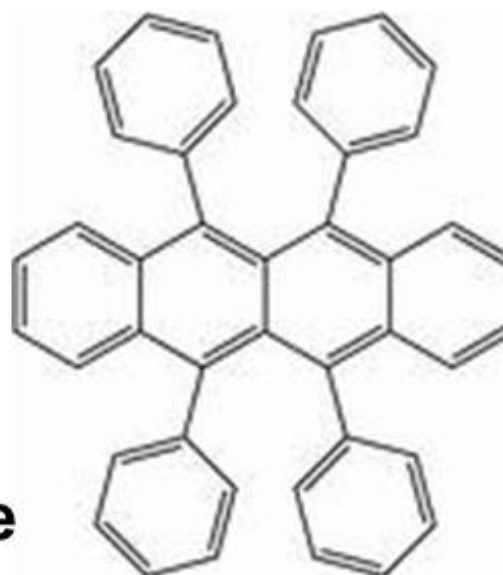
Small molecules

Pentacene

Rubrene

PC$_{60}$BM

OCH$_3$

Polymers

CH$_2$(CH$_2$)$_6$CH$_3$

S

n
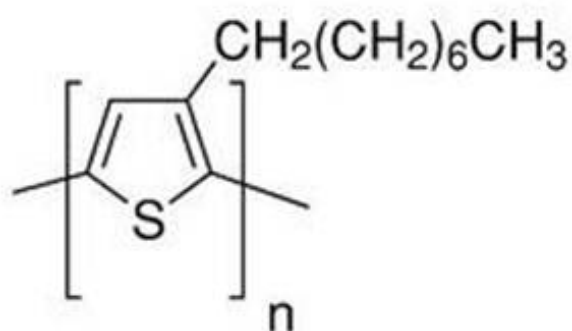
poly(3-hexylthiophene)

n
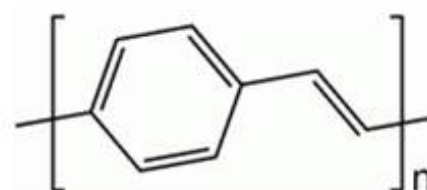
poly(p-phenylene vinylene)

n

polyfluorene

Organic semiconductors

Advantages	Disadvantages
Inexpensive	Low charge mobility
Easy to make	Poor crystallinity
Light weight and flexible	Degradation
Possibility to modify	

T

Organic semiconductors

Advantages	Disadvantages
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T

(a)

https://www.researchgate.net/publication/

275467169_Hydrostatic_pressure_effects_on_structural_and_electronic_properties_of_pentacene_from_first_principles_calculations

6

Lederer et al. (2019)

Link to download the paper:
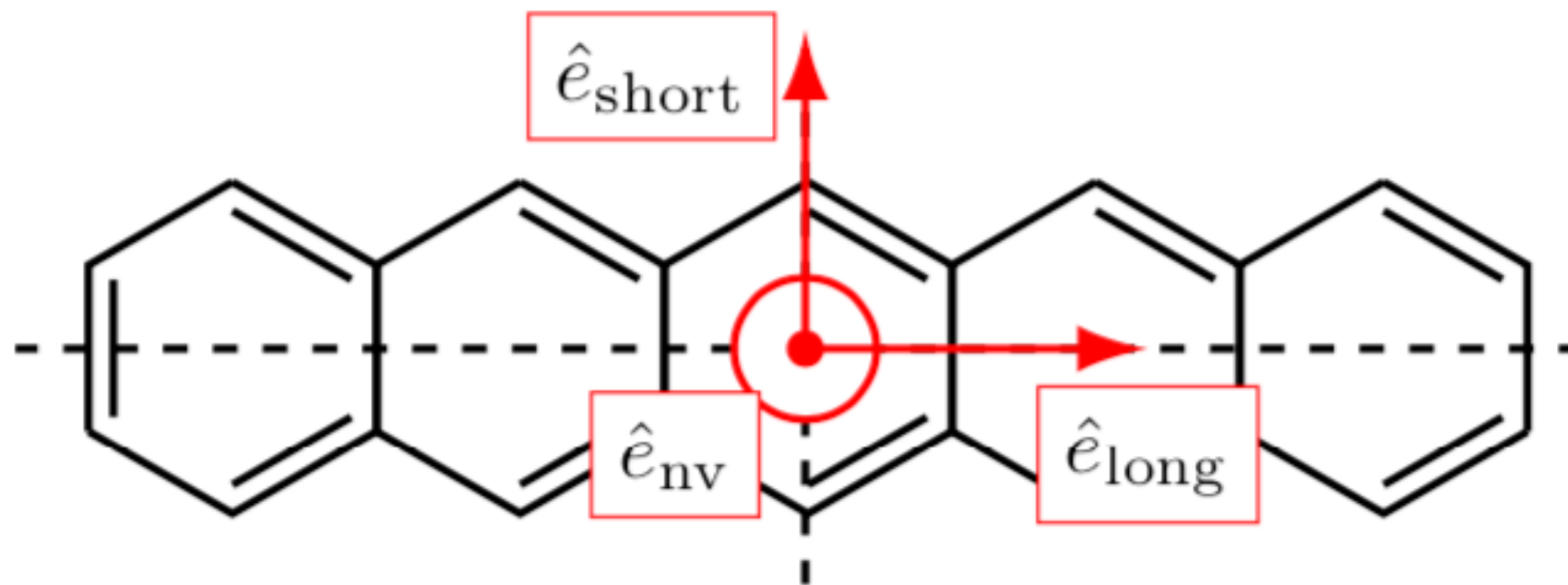
https://onlinelibrary.wiley.com/doi/epdf/10.1002/adts.201800136

Machine Learning–Based Charge Transport Computation for Pentacene, Adv. Theo. Sim (2019)

10

Machine Learning–Based Charge Transport Computation for Pentacene

Jonas Lederer, Waldemar Kaiser, Alessandro Mattoni, and Alessio Gagliardi*

Insight into the relation between morphology and transport properties of organic semiconductors can be gained using multiscale simulations. Since computing electronic properties, such as the intermolecular transfer integral, using quantum chemical (QC) methods requires a high computational cost, existing models assume several approximations. A machine learning (ML)–based multiscale approach is presented that allows to simulate charge transport in organic semiconductors considering the static disorder within disordered crystals. By mapping fingerprints of dimers to their respective transfer integral, a kernel ridge regression ML algorithm for the prediction of charge transfer integrals is trained and evaluated. Sinc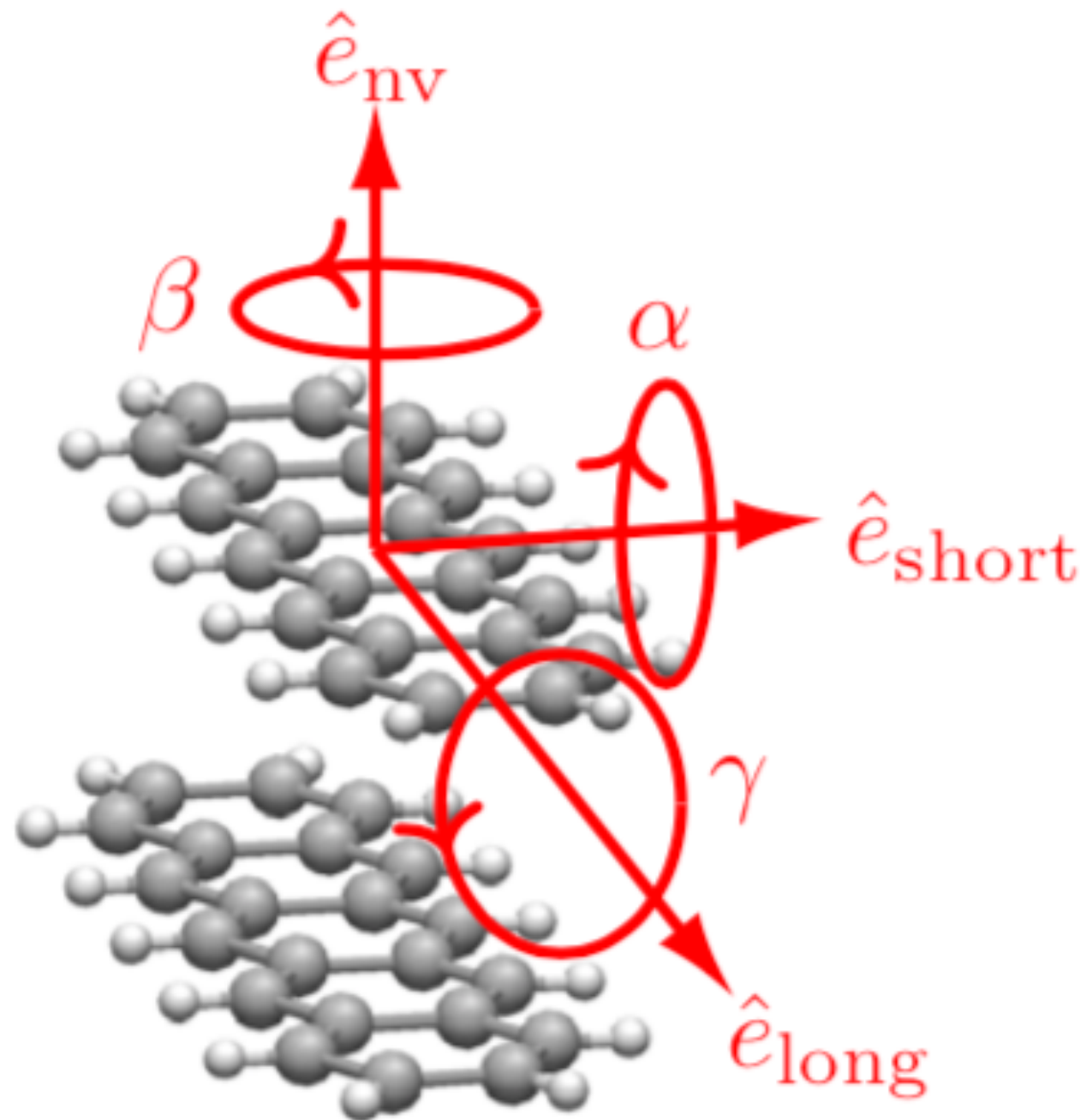e QC calculations of the electronic structure must be performed only once, the use of ML reduces the computation time radically, while maintaining the prediction error small. Transfer integrals predicted by ML are utilized for the computation of charge carrier mobilities using off-lattice kinetic Monte Carlo (kMC) simulations. Benefiting from the rapid performance of ML, microscopic processes can be described accurately without the need for phenomenological approximations.

However, to this day, the main issue concerning organic semiconductors is the low charge carrier mobility compared to their inorganic counterpart,[5] which limits the operational speed and performance of electronic devices. Largest measured mobilities are in the range of $10 \, cm^2 \, V^{-1} \, s^{-1}$ for highly crystalline pentacene[6] and rubrene.[7] Due to the lack of insight into the structure–properties relationships, the design of new materials often relies on chemical intuition. This makes it difficult to identify promising materials with enhanced mobility. Thus, theoretical and numerical models are considered as promising pathways to increase the understanding of the relation between charge transport properties and structural morphologies within organic materials at the nanoscale.[8]
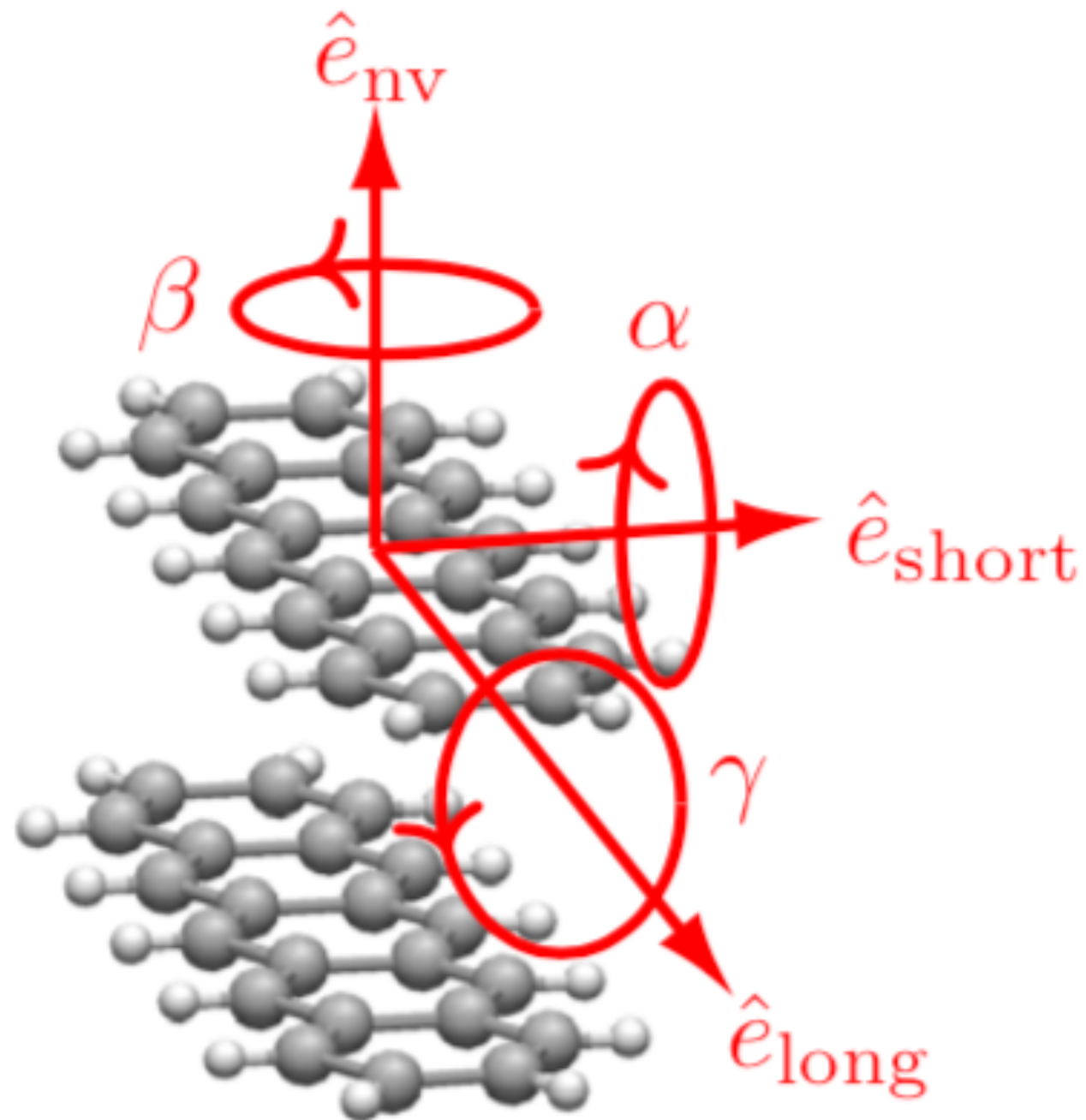
Machine Learning–Based Charge Transport Computation for Pentacene, Adv. Theo. Sim (2019)

11

Features

x, y, z

α, β, γ

Features

x, y, z

α, β, γ

Transfer integral (V_{ij})

T